Phenomena-based Uncertainty Quantification in Predictive Coupled-Physics Reactor Simulations

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

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Phenomena-based Uncertainty Quantification in Predictive Coupled-Physics Reactor Simulations

NEUP Final report

Texas A&M University
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I Background
This project has sought to develop methodologies, tailored to phenomena that govern nuclear-reactor behavior, to produce predictions (including uncertainties) for quantities of interest (QOIs) in the simulation of steady-state and transient reactor behavior. Examples of such predictions include, for each QOI, an expected value as well as a distribution around this value and an assessment of how much of the distribution stems from each major source of uncertainty. The project has sought to test its methodologies by comparing against measured experimental outcomes.

The main experimental platform has been a 1-MW TRIGA reactor. This is a flexible platform for a wide range of experiments, including steady state with and without temperature feedback, slow transients with and without feedback, and rapid transients with strong feedback.

The original plan was for the primary experimental data to come from in-core neutron detectors. We made considerable progress toward this goal but did not get as far along as we had planned. We have designed, developed, installed, and tested vertical guide tubes, each able to accept a detector or stack of detectors that can be moved axially inside the tube, and we have tested several new detector designs. One of these shows considerable promise.

II Delays
This project got a late start and suffered several further delays. The funding award was more than $100k lower than the proposed budget, and compounding this, our original budget was based on a misinterpreted quote for in-core neutron flux detectors, which reduced available funds by another $180k before the project started. As the proposed project was already exceedingly ambitious for the proposed budget, the effective reduction of $280k forced a thorough re-thinking of our data-collection strategies. This included accepting significant risk that our self-developed and self-constructed small incore detectors might not achieve sufficiently mature capability by the end of the project to deliver the data that was originally envisioned. After re-scoping and re-planning, we submitted a revised proposal and budget, and the project began on Nov. 28, 2011.

During the second project year (“PY2”) there was a radical turnover of personnel at our reactor facility, the Nuclear Science Center (NSC). The NSC Director, who was also the project Co-PI responsible for detectors and experiments, was replaced with an interim Director, who was not a detector expert. In PY3 the interim director became the director but subsequently left the
university and was replaced by another interim director. These changes caused the project significant delays and caused us to once again re-think our detector strategy and look elsewhere to secure the required detector expertise. We requested a no-cost extension during Y3Q4 and it was approved in early October 2014. In December of 2014 (Y4Q1), Dr. Sean McDeavitt was named NSC Director, and stability returned to the NSC.

In December of 2014 our department was required to move out of the building it had occupied for decades, into scattered temporary quarters, where we remained until December, 2015, when we moved into a renovated building. The double move was disruptive and took key personnel away from our research project. As part of the moving process, Dr. Delia Perez-Nunez, who was centrally involved in the in-core detector effort, was given significant responsibilities for moving a large radioactive-material laboratory from its long-time home to a different building several miles away, because the long-time home was being demolished. Moving radiation-lab equipment is tedious and time-consuming, and the new facility required modification before it could house and operate the laboratory. This took Dr. Perez-Nunez away from our project for many months. Dr. Adams, the Lead PI, served as the department’s point of contact for renovation of the building into which our department ultimately moved. This took Dr. Adams away from the project and contributed to his being late with reports. In addition, when a Nuclear Engineering professor departed for a different university in May, 2015, Dr. Adams agreed to take over as advisor for two “orphaned” graduate students and also stepped in to help stabilize an Institute that had been directed by the professor who left. These new responsibilities took time, and as Dr. Adams’s time was already fully committed, some commitments had to be deferred. Because of these and other delay-inducing circumstances, in fall 2015 we requested a second no-cost extension through August of 2016, which was granted.

Thus, this project received three years’ worth of funding and attempted three years’ worth of effort, but it was spread over four years plus a portion of a fifth year.

### III Summary

In the sections that follow, we describe the significant advances that we made during this project in the areas of incore detection systems (Section IV), physics-based uncertainty quantification (Section V), neutron transport simulations (Section VI), heat-transfer and fluid-flow simulations (Section VII), and coupled simulations (Section VIII). We did not achieve all of the rather ambitious goals of the project, but progress was significant on every front. We ended the project well positioned to combine the newly developed capabilities with further advances to achieve future results that will significantly advance the state of the art in predictive science and engineering for nuclear reactor analysis.

### IV Incore Detectors

A key task in our project has been to design, analyze, build, and install an in-core instrumentation capability that can produce the validation-quality data the project has aimed to acquire. This has involved several sub-tasks, including:

1. Designing the in-core instrumentation tubes and related hardware that will enable movement of detectors to desired locations;
2. Developing a safety analysis for the in-core tubes (which displace coolant), gaining approval to operate with the tubes in place from the Texas A&M Reactor Safety Board and the Nuclear Regulatory Commission;
3. Designing, building, and testing the system of computers, storage devices, and other electronics that allow accurate inference of interaction rates in neutron detectors, with high resolution in time (sub-millisecond) and high dynamic range (>4 orders of magnitude);
4. Designing, installing, and testing the in-core detectors themselves.

IV.1 In-Core Instrumentation Tubes.

We decided early on to place our in-core instrumentation tubes at corner intersections of four-element fuel bundles (and not, for example, in the central channel of a four-element fuel bundle). This was partly driven by the configuration of our bottom core plate, which has a diamond-shaped opening at each such intersection that can serve to hold the bottom of each tube in place. We considered tube designs with outer diameters ranging from 0.5 to 0.75 inches and eventually settled on an outer diameter of approximately 0.5 inches, which displaces less water and has less effect on neutronics and thermal-hydraulics compared to larger tubes. Jan Vermaak of the Texas A&M Nuclear Science Center (NSC), who became an employee after this project was already underway and subsequently joined the project, led a successful effort to design, analyze, build, and test a hardware fixture that mounts on upper core structures and holds a row of six hollow guide tubes (O.D. 0.5 in.) in place between two rows of fuel in the TRIGA core. Figure 1 shows a schematic of the hardware assembly, and Figure 2 presents a photograph of the assembly. Testing confirmed that an experienced operator can quickly put the assembly of tubes in its proper location, in spite of its resting place being more than 20 feet below the water’s surface.

Figure 3 illustrates how the guide-tube assembly mates with the existing hardware at the top of the TRIGA core. The figure shows a single guide-tube assembly (blue-gray in color) resting on the handles of the fuel-bundles (olive-gray in color) at the ends of the first and second fuel-bundle rows. The tops of the six guide tubes are visible, and much of the nearest guide tube can be seen between the first and second fuel bundle. Each bundle is a 2x2 array of fuel pins, so the tubes in the illustration are between the second and third rows of fuel pins. (Dark gray blocks left and right of the core are graphite.)

Figure 4 is a top view of four guide-tube assemblies in place in the core, with six guide tubes in each assembly. Variation B has its support legs set farther inboard than Variation A, so the two variants can simultaneously support rows of guide tubes next to adjacent fuel-bundle rows. A third variant would be required to fit in the neighborhood of the regulating rod if this is ever needed.
Figure 1. Schematic of the guide-tube assembly that rests atop the core and supports six guide tubes between two rows of fuel.

Figure 5 illustrates how the guide tube, 0.5 inches in outer diameter, fits in the coolant channel at the intersection of four fuel bundles. This figure shows portions of four fuel pins (the large circles), with each pin shown belonging to a different 2x2 bundle. It shows the rectangular lattice of the TRIGA core, with pin-to-pin spacing in $x$ and $y$ equal to 1.66 and 1.51 inches, respectively. The bottom foot of the guide tube is not shown. It holds the bottom of the guide tube in place by making contact with each of the diagonal surfaces of the four surrounding bundles at the bottom of the core.
Figure 2. Photograph of guide-tube assembly, with an early prototype of an in-core detector inserted into third tube from the left.

Figure 3. Schematic of one guide-tube assembly resting atop the TRIGA core.
Figure 4. Schematic top view of four guide-tube assemblies resting atop the TRIGA core.

Figure 5. Cross section of guide tube and flow path at intersection of four bundles.

IV.2 Safety Analysis and Testing of In-core Instrumentation Tubes

During Y2 we completed the safety analysis required before tubes could be inserted into the reactor and were preparing the associated “50.59” document for review by the Texas A&M University Reactor Safety Board (TAMU RSB) when we made the decision to reduce tube
diameters. Calculations were repeated and results re-analyzed. During Y3 we submitted our 50.59 analysis of the reduced-diameter tubes to the TAMU RSB. The RSB approved this in October of 2014. Some of the analysis is described in a paper presented at the 2014 international conference on Physics of Reactors (PHYSOR 2014, late September, Kyoto, Japan).\(^1\)

During Y4 we continued analyzing the effects of the in-core guide tubes, including effects on heat transfer, fluid flow, temperature distribution, power distribution, and criticality. We also completed a series of tests at power, including tests during pulsing operations. Much of this work is summarized in a paper that was presented at the ANS Winter Meeting in November, 2015.\(^2\) Some key findings were:

- The TRIGA reactor is strongly under-moderated, which means that any displacement of moderator will have a negative reactivity and will reduce moderation and power locally. The overall neutronic effect of inserting guide tubes was that the power distribution within the core improved slightly (lower power peaks) since the change in the total effective moderator was higher for internal (high power-peaking) elements than those on the core periphery, mostly because of the outer element’s proximity to reflector material.
- With every-other inter-bundle channel containing a guide tube our analysis found that the total reactivity worth was \(-0.72\), with individual detector movements less than \(0.10\). Such reactivity values are with the technical specification limits of the reactor.
- The three-dimensional effects of the support tubes were evaluated using a CFD model of an entire bundle. The simulation showed no significant change in cladding temperature provided that every-other coolant channel was used for a tube and detector. This was attributed to the inverse proportional relationship between mass flow and coolant velocity, i.e. even though the obstructed channel had less mass flow, the smaller cross-sectional area caused an increase in cooling velocity. See Figure 6 and Figure 7.

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For the evaluation of the Minimum Departure from Nucleate Boiling Ratio (MDNBR) a transient simulation was performed using the RELAP5/MOD3.3. For steady state operation, the margin to a DNBR of unity remains sufficient. Pulse operation was not addressed in the 2014 paper.

After installing the support structure in the reactor core we executed a number of qualification tests. One of the support tubes was located next to an instrumented fuel element. This element showed the same marginal change in centerline fuel temperature—only a few degrees—as predicted by the CFD and RELAP simulations.

During Y4, in addition to further analysis of effects on heat transfer, fluid flow, temperature distribution, power distribution, and criticality, we completed a series of tests at power (including pulsing operations) to verify that we understand the effects of the guide tubes and that they are benign.
During the final partial year of the project (Y5), we added the following:

- Manufactured additional detector support structures (each containing multiple detector guide tubes and associated structural hardware), enabling more locations to collect data simultaneously.
- Tested guide tubes and support structure between control rods and found it to pose no risk to geometrical interference, reactivity or core cooling. (Previous tests were away from control rods.)
- Tested guide tubes and support structure under reactor pulsing, to maximum allowed pulsing reactivity, with no problems arising.
- Performed several design/test cycles to alleviate a water-inleakage problem that we had discovered in what should be dry tubes inserted into the instrument guide tubes. The new tubes appear to be water-tight.

By the end of the project we were satisfied with our in-core instrument guide tubes, which appear to meet all objectives.

**IV.3 Detector Electronics**

Electronics development for our project was challenging, as we knew from the beginning. Off-the-shelf electronics available five years ago did not meet project requirements. We decided early on to forego conventional analog-circuit processing and make the leap to digital, judging that modern A/D converters had progressed sufficiently that we could achieve the necessary temporal resolution and dynamic range, and that the benefits of going digital would outweigh the costs and uncertainties associated with blazing a new trail. This proved to be a sound decision.

We observe that many other groups are now also migrating to A/D conversion and digital signal processing for radiation-detector signals.

We originally determined that a throughput of 250 Msps (million samples per second) and 16 bits per sample would suffice for our data acquisition system. As the required A/D convertors were relatively new in the early phases of the project, we had difficulty procuring evaluation boards and chips. However, we eventually obtained systems from both Analog Devices and Texas Instruments, with the A/D from each company in a module that costs roughly $300. We acquired standard inexpensive PC systems with high-speed generation-3 PCI express, which is a serial standard exceeding 6 Gbps per channel. We could then move data from an I/O A/D card to the PC main memory and then to a SATA III drive at rates exceeding 500 MBytes per second. An inexpensive disk storage system was designed using five standard 3 TB drives. Each drive has a minimum of 100 MB/s sustained read or write, and thus, spreading the data across five drives can achieve over 500 MB/s sustained rates. Through careful system design and in-house integration we have kept the cost of this next-generation data acquisition and storage system to only two or three thousand dollars.

By the end of the first project year we had assembled a 19” rack-mounted system with an open-source Linux operating system. The box includes power supply, fans, a motherboard having PCI express 3.0, SATA III disk controllers, and 10 Mb ethernet. It also has a five-bay unit of SATA III drives with each drive holding 3 TB and sustaining a 100 MB/s data transfer rate. For data acquisition the system will be using FMC-format A/D convertor cards attached to an Xilinx.
FPGA-based PCIe board. Each box will have one Xilinx board and one FMC card, and will be able to handle one or more detectors. The system can digitize a single detector channel at up to 250 Msps at 16-bits. The total disk storage allows several hours of transient data recording. We are currently using a Xilinx prototyping board for DSP applications, which includes two FMC connectors, an FMC A/D & D/A card, and an ethernet connection. At the end of the first year we had all the pieces assembled for an operational, inexpensive, next-generation data acquisition and storage system.

During Y3, testing of the A/D and capture board determined that it did not perform as well as our system required. A more advanced A/D and capture board was ordered and the cabling to carry signals from in-core detectors to the data-acquisition systems was designed.

In Y4 we demonstrated that measurement of counting data at approximately 200 Mhz. This rate of data acquisition carries a high computing cost, requiring multiple solid state drives to handle the enormous incoming data stream, as described previously.

The student involved in the detector-electronics work, Sophit Pongpun, finalized her dissertation during Y5, then successfully defended her work and completed all degree requirements.

**IV.4 Development and Testing of Incore Detectors**

**IV.4.1 Detectors employing boron layers inside tubes**

During the first three years in which the project was active, we iterated on the design of the instrument guide tubes and a basic detector that would fit inside them. The detector employed boron layers (a “boron straw”) on the inside of a small cylindrical tube with anode wires along its axis. The outer surface of the detector tubing was designed come in contact with coolant inside the guide tubes, but the top of each detector tube had electrical connections that remain dry. This is accomplished via a water-tight seal from the top of the detector tube to a larger-diameter insertion tube that not only housed the cabling from the top of the detector to the signal-acquisition system but also provided a sufficiently rigid structure that an experienced operator could steer the detector tube into any guide tube previously inserted into the core. Six detector tubes (designed for insertion into guide tubes) were fabricated.

Figure 2 (in a previous subsection) shows a boron-straw detector tube, with the detector hardware and electronic connectors installed, inserted into an incore guide tube. Figure 8 depicts the bottom portion of a boron-straw detector, with dimensions shown. Figure 9 illustrates both top and bottom ends of the detector in its tube, and Figure 10 shows some of the detail of the top end. Figure 11 provides two views of the top cap including cable penetrations.
Figure 8. Schematic of bottom end of boron-straw detector.

Figure 9. Schematic of boron-straw detector inside its tube, showing top (left side) and bottom (right side).

Figure 10. Schematic showing detail near the top of the boron-straw detector.
The original boron-inside-tube design exhibited significant electronic noise generated by “microphonic” vibrations. Testing and refinement were unable to reduce this to acceptable levels while remaining within the 0.5-inch guide tube. When we first encountered the microphonic noise problem, we started a contingency effort, described in the next sub-section, and by the end of the third year the contingency boron-on-copper concept had become the main focus of our in-core detector development effort. Near the end of the project we devised an even more promising approach—home-made self-powered neutron detectors—which we describe in a later sub-section.

IV.4.2 Detectors with boron on copper

During Y3 we launched a second detector-development effort as a contingency against the possibility that the microphonic noise in the original design might prove insurmountable, which turned out to be the case. The second effort pursued a high-risk/high-reward strategy looking at novel concept with the potential to address the unusual dynamic-range requirements of our project—requirements that are driven by the desire to accurately measure neutron flux levels that change by six orders of magnitude on a sub-second time scale during a fast pulse. The second detector development effort is coupled with an electronics effort that miniaturizes the HV power supply and preamplifier, placing them onto small printed circuits that are deployed in a dry tube deep in the pool only a few feet from the reactor, thereby avoiding multi-meter cable runs from the detector, which would degrade the fidelity of the pulse shape coming from the detectors.

The proposed concept is coaxial, with a central conducting wire surrounded by air contained in a high-purity copper cylindrical shell, with a small window in the copper for boron. The idea is to count pulses from the charged particles that result from neutron interactions with the boron, and to have the pulse rate low enough that the detector maintains sensitivity even at the peak of a reactor pulse (when power reaches several hundred MW and fluxes exceed $10^{15}$ n/cm$^2$-s).

The detector’s requirement for low response rate at high neutron flux was largely born from its requirement to measure reactor pulses where the rapid redistribution of flux is of particular interest to reactor analysis code developers. In order to achieve such a low sensitivity, a very
small ion chamber was used. A $^{10}$B layer was placed outside of the cathode tube instead of on the inside, which allowed a 0.1 mm projection hole to be made in the side of the cathode tube. This allowed a large reduction in the rate of $\alpha$-particle (and Li-particle) production without sacrificing ion production volume. This effect can be seen in Figure 12. The overall design is depicted in Figure 13.

![Figure 12. Particle tracks ($\alpha$ and Li) inside the mini ion chamber.](image)

During Y3 we obtained prototypes of thedeployable circuit boards that measure 0.6 inches wide by 12 inches long. Preliminary testing of the boards, coupled with 90 feet of cable to take the pre-amp output from near the core all the way to the data-acquisition racks, began during the later part of Y3. During Y4 we executed several design/test/re-design iterations, with tests ranging from table-top with alpha sources to in-core, using dry tubes inserted into the in-core guide tubes referred to above.

![Figure 13. A sketch of the thermal neutron detector (not to scale). The detector is made from a high-purity copper anode wire and a high-purity copper high voltage tube with a 2-mm hole lined with B-10.](image)
The system responded as expected when tested with an alpha source, a gamma source, and in the reactor. For in-core testing the detector was inserted into 30-foot hollow tubes (intended to be dry) and tested with the reactor at low powers, in the range of 50 W to 100 kW. In spite of problems with water leakage into what should have been a dry tube, we verified that detector was working and the electronics and data acquisition system performed well. MCNP calculations were performed to help untangle the effects of gamma-induced interactions from neutron-induced interactions. It soon became clear that gamma interactions cause a high background in the boron/copper incore detectors that can make it difficult to extract the desired neutron signal with the desired precision, even with digital processing of signals collected at several hundred Msps. After analysis and testing we decided to pursue a “compensated” design in which two almost-co-located detector volumes are used, one with and one without boron, with the two signals subtracted to eliminate the gamma signal.

The design and testing of the uncompensated detectors and associated electronics was described in a student paper given in the NEUP-Sponsored-Student session at the ANS Winter Meeting in Washington, DC, in November of 2015.3

During the final partial year of the project we completed an initial design of our compensated boron-on-copper detector system. This required not only a new detector system but also modification of the high-voltage power supply, which was originally designed to generate negative high voltage for the uncompensated boron-on-copper detector. The power supply was modified in to supply both positive and negative high voltage, as needed by the gamma-compensated born-on-copper detector system. The circuit was further modified to support different modes of operation that may be needed when neutron flux is very high. The circuitry was modified to allow jumps in current from micro-amps to milliamps without a large drop in HV output. This is needed (as the HV current equals the ion current due to neutron detection) to allow transient behavior with millisecond resolution, as the HV cannot regulate that quickly to account for severe HV drop due to changes in current draw. As the boron-on-copper system uses ion chambers and not proportional tubes with gain, this only modestly effects the ion transit time and rise time of the preamp signal. As we directly measure preamp output and not the shaped output, this will not affect the neutron measurements, as the same basic charge will be deposited (just over a slightly longer period). We account for this by examining the preamp signal over a slightly longer time for pulses (and for current mode it doesn't matter). This is readily done with digital processing. The HV supply also now has a circuit to measure current. Finally, we developed a difference circuit to subtract the first chamber’s current, which is due to gamma interactions, from the second chamber’s current, which is due to both gamma and neutron interactions, yielding the current due to neutrons only.

During Y5 we constructed our first compensated boron-on-copper/just-copper detector pair deployment in our incore instrumentation guide tubes. The detector has two chambers, which have identical dimensions and share a grounded anode wire. Only one of the chambers has boron

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to capture neutrons and its wall is connected to a negative high voltage. The other chamber does not have target material for slow neutrons and is connected to a positive high voltage.

A photograph of the newly constructed detector is shown in Figure 14 below, and a sketch of the detector that was initially designed earlier in Y5 is shown in Figure 15. Compared with the original design, in the as-built detector the chamber with boron is moved to the end of the detector, which simplified construction and further modification.

Figure 14. Prototype of compensated boron-on-copper detector.

Figure 15. Design schematic, preliminary design of compensated boron-on-copper detector
During Y5 we completed a paper that was presented at the 2016 PHYSOR conference.\textsuperscript{4} This paper describes our detector and data-acquisition systems and how they are designed to provide excellent time resolution during rapid transients, such as pulses in our TRIGA reactor. Also during Y5 we demonstrated that our understanding of the incore detectors is sufficiently complete that our simulated detector responses agree well with the measured data. This is illustrated in Figure 16 and Figure 17 below.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{simulation_graph.png}
\caption{Simulated response of incore detector.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{measurement_graph.png}
\caption{Measured response of incore detector.}
\end{figure}

IV.4.3 Self-Powered Neutron Detectors

As the project was ending, some project team members began exploring self-powered neutron detectors (SPNDs) as candidates for our in-core detectors. On first consideration SPNDs may seem too expensive for projects such as ours, but it appears that with our electronics system already in place, we may be able to construct SPNDs ourselves very inexpensively, with results that may meet all of our goals, including wide dynamic range, rapid time response, low gamma sensitivity, and predictable current output as a function of neutron capture rate in the small detector volume. We ran out of time and resources on this project before we could get very far with this detector concept, but we did manage to build a prototype and collect some data, as we describe here.

With an SPND, an insulated portion of the detector becomes charged (usually positively) and can then be used to drive a current. The term self-powered refers to the detector not requiring a high-voltage source. In the context of cobalt detectors, which is the basis for our prototype, the detection process utilizes the prompt \((n,\beta)\) reaction of natural Cobalt. We sought to meet the following requirements:

- Wide dynamic range—should respond at low reactor power as well as extremely high powers (>1000 MW)
- Must be robust (can not easily break, misalign or burn up)
- Should provide a continuous signal rather than be event-based pulses
- Should be fairly gamma insensitive (enough to distinguish power level changes at low neutron fluxes)

In order to maximize the current at low fluxes a 4 mm diameter Cobalt rod was used as the core material, polyethylene-insulated, with a collector constructed from a thin aluminum tube having an outer diameter of 10.67 mm. Final length will vary between 19 and 25 mm, which would allow us to fit 15 detectors axially in a single instrumentation tube along the height of the active core. Our prototype detector is pictured in Figure 18 below.

![Figure 18. Cobalt detector prototype with collector and polyethylene insulator removed.](image-url)
Because of the prompt reaction, the detector response time is on the order of $10^{-8}$ s. Current source strengths of 0.54 microamps at a thermal neutron flux of $10^{14}$ n.cm$^{-2}$.s$^{-1}$ is achievable.

Figure 19 shows the detector output current (in nano-amps, on the right-hand vertical axis) as a function of reactor power (left axis), with the power number coming from the reactor’s Compensated Ion Chamber (CIC). For this test the SPND was not connected to a pre-amplifier and was placed on the west face of the core in a nominal irradiation position dry-tube. The output current was measured with a pico-ammeter. The gamma-radiation noise level (from decaying fuel elements) is seen to be approximately equivalent to a reactor power of between 3 and 6 kW.

Figure 19. Cobalt SPND detector current output at different reactor powers. (Current measured with a pico-ammeter; power inferred from reactor’s compensated ion chamber.)

The plot shows that the detector outputs a current high enough (above the gamma noise signal) to indicate the difference between source-range (~1 W) and initial critical power (300 W). This is important because reactor pulses are performed from power less than 1000 W. At higher powers the output current becomes notably less noisy and the ability to capture fast transients is apparent.

A logarithmic amplifier was connected to the detector to measure the logarithmic equivalent of the current during a reactor pulse. This also converts the signal to volts. The logarithmic amplification was necessary because the nominal low power signal is approximately 1 nA ($10^{-9}$ A) and with a linear amplification, to bring the low voltage above the noise threshold, the expected current during pulses of $\mu$A will likely exceed the capability of any operational amplifier.
The log-amp output was then connected to a buffer with sufficient impedance to allow connection to the very low impedance and very high acquisition rate of the acquisition card. This arrangement unfortunately enhanced noise and did not allow for break-through signal higher than a power equivalent of approximately 10 kW.

Figure 20 and Figure 21 show the measured values during a pulse. As can be seen on the logarithmic plot, there is a significant level of noise at lower power levels. This problem can be eliminated with more precise electronics (this test used a quickly developed prototype) as well as being in regions of higher flux. The ionization chamber used for the pulse-power monitor channel is shown in orange and is very noisy but only used for higher power levels. A reference adiabatic point-kinetics calculation (with similar thermal feedback coefficients) is also shown in the plot. From this plot the detector setup (which currently is not ideal) does show a response above 10 kW, however, it is not the correct response and prompted an investigation into the logarithmic linearity of the amplification circuit.
To investigate the input vs output characteristics, a calibrated current source was used to supply specific signals to the amplification circuit (i.e. log-amp plus buffer arrangement). The response curve is shown in Figure 22. From this plot one can also see the expected linear response and its significant deviation. This effect can definitely be improved with a better circuit design but for now a data compensation was manually performed.

Figure 22. Measured response of amplification circuit (not the SPND itself) showing that the quickly assembled circuit is the source of the observed nonlinearity.

A corrected signal is shown in Figure 23 and Figure 24. This signal is derived by applying the deviation factors obtained from Figure 22. The response is much more realistic, but shows amplification of the low-current noise problem, for which a solution will need to be sought.

Figure 23. Detector responses (compensated ion chamber and new SPND corrected for amplification-circuit nonlinearity) during a pulse: log scale.
When the project ended, there remained several issues that need to be resolved before our simple, low-cost SPNDs can be trusted to generate validation-quality data. These include:

- The amplification circuit requires higher frequency response and overall better performance.
- Components need to be used that are less noisy (ranging from connectors and cables to op-amps and circuits).
- The detector is NOT insensitive to gamma (fortunately a lot of literature is available to help address this).
- If we filled all of our potential instrument-tube locations to obtain a time-dependent full-core flux map, we would have approximately 5 rows by 6 columns by 15 detectors stacked axially in each tube, resulting in 450 sensors. Each would need a signal cable and acquisition channel. This will require some engineering to make it compatible with reactor operation.

IV.4.4 Summary of Detector Effort

By the time the project ended, our detector development and deployment effort had recovered from previous disruptions at the Nuclear Science Center and was making excellent progress toward an inexpensive, reliable system of incore detectors and associated analog and digital electronics that could produce the validation-quality data that we are all eager to obtain. We succeeded in developing and deploying a new signal-acquisition-and-analysis system based on low-noise analog electronics, analog-to-digital conversion at rates in the hundreds of MHz, and rapid storage of massive digitized data. We had not completed the task of developing and deploying an array of incore detectors, but we had explored many potential designs and made significant progress. In particular, our small, inexpensive, home-made SPNDs show great promise. Our students and early-career researchers gained valuable experience and knowledge in detector design, signal acquisition, and signal analysis throughout the process.
V Uncertainty Quantification

Much of our work in the Uncertainty Quantification (UQ) arena is well documented in a series of publications. In this section we summarize much of this but refer the reader to the publications for the details.

V.1 Uncertainties in Cross Sections

An important component of a complete UQ treatment of a reactor-analysis problem is assessment of sensitivity of calculated quantities of interest (QOIs) to uncertainties in cross sections. During this project we made significant progress with our adjoint-based approach to this task.

Proper treatment of cross-section uncertainties requires knowledge of how the uncertainties in various cross sections are correlated. The basic characterization of this can be expressed in a covariance matrix. Our team has developed scripts (now included in the “barnfire” cross-section processing system that we developed during the course of this project, described below) to generate covariance data using NJOY2012. NJOY2012 can calculate multigroup covariance data for arbitrary energy discretizations and arbitrary collections of nuclides. This is essential for UQ studies for neutron transport calculations in reactors.

Although multigroup covariance data can be generated with NJOY, the NJOY input files are not straightforward to generate and the covariance data in the NJOY output is not easily accessed. Our “barnfire” scripts make this simpler. In addition, our scripts have the ability to generate not only the “mean” values of cross sections, but to generate randomly sampled realizations of full (multigroup, many-nuclide) cross-section sets from the multivariate Gaussian distribution defined by the mean values of the cross sections and the covariance matrices extracted from the NJOY2012 output. The mean values and realizations of the cross sections can be written in the format specified for a particular radiation transport code, such as our PDT code.

During the course of this project we developed improved techniques for propagating cross-section uncertainties through reactor-analysis calculations, properly accounting for correlations by using co-variance matrices, and thereby obtaining QoI distributions whose spreads are due to realistic treatment of cross-section uncertainties. One key part of this work is a new dimension-reduction (which is essential when there are large numbers of uncertain input parameters, as is the case rather dramatically with cross-section data). Much of this is summarized in a peer-
reviewed conference paper.\textsuperscript{5} A more complete description of the cross-section UQ technique is given in the dissertation of a student who graduated near the end of the project.\textsuperscript{6}

As part of our investigation of the thermal scattering in ZrH\textsubscript{x}, which is a major focus of the project, we encountered idiosyncrasies in the results from the NJOY cross-section processing code. This prompted us to study the behavior of NJOY on a benchmark problem that we developed. We found that for higher scattering moments, the multigroup cross-sections from NJOY can be significantly incorrect and can even have the incorrect sign in a simple, free-gas hydrogen test problem. We published these results in a paper that appeared in 2015.\textsuperscript{7}

\textbf{V.2 Emulators}

During the project we studied the accuracy of “emulators” as surrogates for high-fidelity neutronics calculations in TRIGA reactors. Emulators, built (by sophisticated regression techniques) from results of high-fidelity computations at sets of carefully chosen input-parameter values, are an important part of our overall physics-based UQ effort, and it is important to ascertain how well they approximate high-fidelity results at parameter values that were not part of the training set. We demonstrated that the construction of emulators on full-core simulations of TRIGA reactors can be used to build a surrogate model (aka emulator) to accurately represent MCNP simulation results across the required range of phonon-spectra parameters previously introduced in our parameterized phonon spectrum model. Using the emulator we are able to use a hypothetical experiment (with uncertainties) to calibrate the parameters in the phonon spectrum. This work is described in a journal paper that appeared in 2016.\textsuperscript{8}

Additional work on emulators for reactor-analysis QoIs concerned variable selection and sensitivity coefficients. This was reported in a peer-reviewed conference paper.\textsuperscript{9} An honor’s theses directed by Co-PI McClarren also contributed capabilities that improve the state of the art

\begin{itemize}
\item \textsuperscript{8} W. Zheng and R.G. McClarren, “Emulation-Based Calibration for Parameters in Parameterized Phonon Spectrum of ZrH\textsubscript{x} in TRIGA Reactor Simulations”, Nuclear Science and Engineering, 183, 78-95 (2016)
\end{itemize}
in reactor-analysis UQ, in particular in the realm of inference of physically significant parameters from measured data.\(^{10}\)

**V.3 Depletion**

A key feature of our project is quantification of uncertainties in a variety of measured and calculated values. For example, the neutron fluxes that we calculate will be contaminated to some degree by discretization errors (in the spatial, directional, energy, and sometimes temporal variables) and by errors in the calculated nuclide concentrations. We must estimate the quantitative impact of these errors on the calculated quantities of interest—for example, on the calculated fission rate in a given fission chamber at a given core location during a given experiment.

We have developed an adjoint-based technique for estimating the error in nuclide concentrations that are produced by depletion calculations of the kind that we will perform with PDT. This builds on work reported in journal article\(^{11}\) and conference paper.\(^{12}\)

An important challenge is in handling re-construction and storage of the full forward transport equation during the adjoint calculation. Early in the project, we developed and tested a suite of 4 algorithms for doing so. Later we applied lessons learned and created better algorithms, which were also tested for their RAM and I/O usage as well as their scalability. The initial round of testing was completed in Y2 and was part of Hayes Stripling’s dissertation effort.\(^{13}\) The algorithms and strategies that we developed have proved to reduce memory and i/o demands to acceptable levels while not significantly increasing CPU times. The main trick is to store and/or write only source moments, not full angular fluxes, and then to rebuild fluxes with single transport sweeps as they are needed.

**V.4 Physics-Based ZrH\(_x\) Scattering Model**

During Y2 we continued our effort to formulate the model we will use to calibrate the \(S(\alpha, \beta)\) parameters for thermal scattering in the zirconium-hydride fuel material. The main thrust has been in understanding current state-of-the-art scattering models so we can parameterize them effectively. We succeeded in Y2 in producing realizations of cross-sections from this model.

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putting them into a form that PDT can use in its simulations and performing initial test calculations using them. Work continued on the code in Y2 to allow it to utilize the phonon expansion technique that is used in NJOY to compute thermal scattering cross-sections.

Previously in the project we developed parameterized phonon spectrum (PPS) models that determine scattering kernels for H and Zr in ZrHₓ. We proposed seven parameters to formulate the PPS model and can control the PPS model by varying the parameters. We employed Latin Hypercube Sampling (LHS) designs to sample the parameters over the seven-dimensional input space and used NJOY to generate cross sections based on the sampled parameter sets. We demonstrated that the variations of the parameters of the PPS model can be propagated through the scattering kernels to continuous-energy/multigroup thermal scattering data of ZrHₓ.

We then performed MCNP simulations of a simplified TRIGA lattice model and investigated the reactivity and the fission rate density. The analyses indicated that reactivity is sensitive to the parameters in the PPS model while the fission rate density is insensitive to the PPS model parameters. Analyses also implied that reactivity is most sensitive to the optical mode peak position and acoustic mode branching ratio of H, which we refer to as the “main factors,” in the ZrHₓ bound system.

We later extended our work from the TRIGA lattice to both simplified and detailed full-core TRIGA geometries, again with MCNP. In the full-core model, several quantities of interest (QOIs), including reactivity, effective delayed-neutron fraction, mean neutron generation time, temperature feedback coefficient and detector absorption rates (in-core/ex-core) were studied. ANOVA with cross-validations based on regressions were employed to test the sensitivity of QOIs to the proposed parameters.

An important component of the project was development of a new physics-based parametrization of the phonon spectrum in the ENDF model for thermal neutron scattering in zirconium hydride (ZrHₓ). This model is an improvement over the previous parameterized phonon spectrum (PPS) model in that it makes no simplifying assumptions as to the shape of the phonon spectrum. For instance, PPS approximated the optical part of the spectrum as a Gaussian, whereas the new model is based on perturbing the ENDF phonon spectrum. We used this new model to study how different parameter settings affect scattering, using MCNP simulations of the NSC TRIGA reactor core. During this study we identified errors in NJOY’s calculation of higher scattering moments for thermal neutrons. We showed that higher Legendre moments of multigroup scattering cross sections can have non-negligible errors when compared with other integration techniques. We reported this in a paper that appeared in 2015.7

Our analysis suggests that some QOIs, including reactivity, prompt-neutron lifetime, and fuel temperature coefficient of reactivity, are sensitive to phonon-spectrum parameters, especially those like the “main factors” cited above. This means that when our UQ and inference machinery are ultimately fed by validation-quality incore data, it may be possible to infer details about the scattering laws in the ZrHₓ+U matrix with its relatively heavy loading (30 weight %) of uranium. This is an interesting topic for further study.
VI Neutronics

Our main neutronics task is to develop a neutronics model, using our PDT code, that accurately represents our TRIGA core. One key component of this task is to develop the capability to generated spatial grids that accurately model the complicated reality of our TRIGA and the capability for PDT to run efficiently with such grids. Another key component is to explore, quantify, and reduce to acceptably low levels our numerical error in quantities of interest in problems of interest, as a function of spatial, angular, energy, and temporal discretizations. Yet another key component is to improve the single-core and parallel computational performance of PDT, so that we maximize the useful results we obtain per machine-hour. For any of this to produce useful results, it must use accurate cross sections.

VI.1 Cross Sections

As anyone who has compared particle-transport calculations against experimental results knows, it is important and difficult to obtain the correct material descriptions and cross-section data; to verify that the obtained data is what was desired and does not obtain serious errors; and to manage the large quantities of data in a way that meets project needs. During the course of this project, our research group devoted substantial effort to these data issues, which in our case have two significant “extra” requirements:

1. Data must support our Finite Element with Discontiguous Support (FEDS) energy discretization scheme. FEDS defines and uses cross-section data that differs somewhat from standard multigroup data.
2. Data must include covariances, to enable proper study of uncertainties in QOIs that stem from uncertainties in cross sections.

During the course of this project, our team discovered several problems with the multigroup cross sections generated by NJOY and worked with the NJOY team at LANL to obtain “patches” that resolved the issues. See, for example, a peer-reviewed conference paper that we recently presented at the 2017 ANS Math & Comp Conference, concerning the treatment of thermal motion in generating scattering matrices.14

During the final project year we collected various cross-section processing capabilities into a unified system that we call “barnfire.” The barnfire system includes the following capabilities (among others):

- Barnfire reads an input that contains a list of nuclides, among other things, and then automates the running of NJOY2012 to generate the needed data files.
- Barnfire can generate FEDS data or standard MG data.

• Barnfire supports multi-temperature cross sections, which can be converted from multi-temperature MATXS cross-section format. PDT can read these data and interpolate to get cross sections at any needed temperature.
• Barnfire can obtain covariance matrices from NJOY2012 for correlated cross sections, not just for a single nuclide but also for sets of nuclides that may be correlated (because, for example, one nuclide is used as a reference for inferring another nuclide’s cross sections).
• Barnfire can separate the prompt- and delayed-neutron spectra, which can be important in the analyses of transients.

VI.2 Spatial Meshing

At the start of the project our PDT code could generate a spatial mesh in which a logically-hexahedral grid could be generated such that it conformed to the cylinders of reactor pin cells, as shown in Figure 26. However, at the project’s beginning, this mesh-generation technique in PDT could be used only with serial runs, which significantly diminished its utility. Early in the project we eliminated a substantial amount of old mesh-generation code, much of which did not work in parallel, and replaced it with efficient and extensible parallel code. Soon we could routinely generate and run reactor-grid problems of the type shown in Figure 25–Figure 26.

During Y3 we originally developed strategies for replacing logically rectangular grids with more efficient “spider-web” type ring-and-spoke pincell grids. Later, also during Y3, we revised this plan as follows. Rather than incorporating “spider-web” grids into the existing pincell grid-generation coding we launched an effort to create a more flexible parallel grid-generation system and implement it into our PDT code. This system would allow independent mesh generation to take place in parallel in each sub-domain (which we call a “cell subset”), with the independently generated grids subsequently “stitched” together at subset interfaces. The stitching would take advantage of PDT’s arbitrary-polygon/polyhedron capability. For example, in 2D, if a triangular cell in one subset has two vertices on an interface, and the neighboring subset places a cell vertex on that interface between the triangle’s vertices, that vertex is added and the original triangle becomes a quadrilateral with two of its edges being co-linear.
During Y4 we launched the design, implementation, and testing of this independent-mesh-and-stitch approach. The new system uses “cut planes” to divide an x-y domain into sub-regions that ultimately become “cell subsets” in PDT. Each subset knows about the geometric features that its spatial mesh must resolve and is told via user input how finely the subset should be meshed. In PDT we now have the capability to use the TRIANGLE mesh generator to independently mesh rectangular sub-regions of an x-y plane and resolving arbitrary polygons or planes, and—more importantly—to “stitch” the sub-regions together by adding vertices to triangles that have edges on sub-region boundaries (thus forming arbitrary polygons). In a 3D problem that can be
well represented by polygonal prisms, such as that of our TRIGA reactor, we project all geometric complexities onto the $x$-$y$ plane, generate a polygonal mesh in the plane as described above, and then extrude this polygonal mesh into a 3D polygonal-prism mesh. We allow an arbitrary number of axial planes, each with arbitrary height, and we allow independent material assignments for each region plane by plane. Figure 27 illustrates this capability, showing a slice through a polygonal-prism mesh that resolves a variety of thin cylindrical shells.

Figure 27. Slice through a grid illustrating new polygonal-prism meshing capability.

Later in the project we developed load-balancing algorithms, for problems with irregular structure, in which we adjust the locations of the “cut planes” until we achieve approximately the same number of spatial cells in each cell subset. This greatly improves parallel execution time in problems with irregular features.

Also during the course of this project, our research group developed the ability to read MCNP input files to obtain the required information about geometry, materials, and sources, and then combine this with user directives to generate PDT input files and meshing instructions. By the end of the project the following procedure had become standard for many geometries of interest:

- Apply software developed in our research group to read an MCNP input file’s geometry and materials descriptions, project interfaces into a single plane, and write two files: (1) a 2D meshing and region-definition file, and (2) an “extrusion” file that defines materials and other regional attributes, axial layer by axial layer, for each 2D region;
- Use routines recently developed inside of PDT to read the two files along with a simplified PDT input file, call the TRIANGLE meshing code for each “subset” of the 2D geometry (in parallel), independently for each subset;
• “Stitch” the subset meshes across interfaces, taking advantage of PDT’s polygonal-cell capability to add “hanging” vertices to triangles, converting them into degenerate polygons;
• Extrude the 2D polygonal mesh into 3D polygonal prisms.

An example of a resulting mesh is shown in Figure 28. Another example is depicted in Figure 29. In this figure the water has been made transparent to permit fuel pins and other structures to be observed. The mesh shown is coarse by design, for this was simply a test problem.

Another example of our current meshing capability is shown in Figure 30. Here we have used the TRIANGLE mesh-generation code to generate a grid for a pincell with the cladding resolved. Note that TRIANGLE does not mesh the object uniformly, and it has some trouble with the thin cylindrical shell. We are pursuing alternatives that will overcome these difficulties and hope to report on them in the near future.

Figure 28. Visualization of a PDT mesh of a complex geometry. The geometry represents an experiment in a “dry cell” adjacent to a “window” in the pool that houses our TRIGA reactor. The reactor is meshed, as is part of the pool and portions of structures inside the dry cell. This mesh was generated directly from an MCNP input file supplemented by user-input resolution directives, using scripts that our team has developed for this and other projects.
Figure 29. Example of polygonal-prism meshing capability, which begins with an MCNP input file, uses translation software developed by the project team, and calls the standard open-source code TRIANGLE from within PDT at run time.

Figure 30. Pin cell with cladding resolved, as meshed by TRIANGLE.
VI.3 Energy Discretization

Energy discretization has long been the most difficult issue for high-fidelity deterministic transport calculations of neutronics in reactors. The multigroup method can produce accurate integral quantities of interest, but only if extreme care is taken in generating weighting spectra tailored to the specific regions of the specific problem of interest. Standard multigroup techniques do not produce accurate detailed quantities of interest (such as the absorption rate in $^{238}\text{U}$ in a particular ring of a particular fuel pin), nor do they show convergence to the continuous-energy solution until the number of groups becomes larger than the number of important resonances, which is intractably large for high-fidelity 3D full-core simulations.

During the course of this project, our research team developed a new energy discretization method that combines the strengths of multigroup and multiband (or sub-group) methods along with new ideas. The new method, called Finite Element with Discontiguous Support (FEDS), shows great promise in addressing the weaknesses of previous methods. It yields solutions that show convergent behavior (to the continuous-energy solution) beginning with less than 100 energy groups, and further provides an avenue for estimating energy discretization error. These desirable features are not provided by the standard multigroup (MG) method.

We chose the FEDS methodology, recently developed by our group,$^{15,16,17,18,19}$ for energy discretization in our high-fidelity simulations. Whereas multigroup (MG) partitions the energy domain into contiguous intervals, as depicted in Figure 31, FEDS partitions the energy domain into discontiguous elements depicted in Figure 32. Discontiguous sets of intervals are chosen by a “clustering” algorithm based on how closely the solutions in those intervals are correlated, usually because those intervals have similar cross-section values in materials of interest. FEDS

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uses high-resolution “snapshots” (examples) of spectra from several materials at several locations in pre-defined representative problems to determine its energy mesh.

**Contiguous meshing of the energy domain (MG)**

![Contiguous meshing](image1)

*Figure 31. Multigroup partitioning of energy domain*

**Discontiguous meshing of the energy domain (FEDS)**

![Discontiguous meshing](image2)

*Figure 32. FEDS partitioning of energy domain*

We have demonstrated that FEDS produces a solution that exhibits well-behaved convergence to the continuous-energy solution as the number of unknowns increases, for unknown counts that are orders of magnitude lower than would be required for MG to begin showing such convergence. This is documented in the papers cited above.

A natural consequence of the clustering procedure is that some FEDS cross sections are averaged over energy ranges near the peaks of resonances, which means that some cross sections in a FEDS calculation are quite large. This is not the case in typical multigroup calculations, which have cross sections averaged over contiguous energy intervals containing both high and low cross section values. The presence of high cross-section values in the FEDS parameters allows the calculation to correctly resolve surface-layer phenomena, such as the production of $^{239}\text{Pu}$ in the outer rim of uranium fuel, which is important for high fidelity. However, this places greater stress on spatial meshing and discretization methods, which now must resolve boundary-layer behavior. During the final project year we explored the spatial, angular, and energy resolution needed to obtain high-fidelity deterministic solutions to thermal-reactor problems when FEDS is the energy discretization methodology. Some results from PWR-type problems are documented in a paper that was presented at the PHYSOR 2016 conference. Some results for a two-dimensional TRIGA pin cell are given below in Table 1. These calculations were performed with a FEDS cross-section set that had 244 degrees of freedom, with standard multigroup used for energies above 20 keV and below 1 eV. The calculations employed 4 polar angles per hemisphere, using “product” Gauss-Chebyshev quadrature sets with varying numbers of azimuthal angles per octant, as shown in the table.
Table 1. Error = (PDT k) – (finely resolved PDT k), in pcm: TRIGA pin cell

<table>
<thead>
<tr>
<th>Cells per pincell</th>
<th>Azimuthal angles per octant</th>
</tr>
</thead>
<tbody>
<tr>
<td>196</td>
<td>256</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>-67</td>
<td>-6.3</td>
</tr>
<tr>
<td>-80</td>
<td>-23</td>
</tr>
<tr>
<td>-79</td>
<td>-21</td>
</tr>
</tbody>
</table>

The calculational flows that produce FEDS cross-section data are given below in Figure 33 and Figure 34. More detail can be found in the references cited above.

Figure 33. Overall calculational flow for FEDS cross sections.
Figure 34. Calculational flow within NJOY during FEDS cross-section generation.

Estimation of numerical error relies on well-behaved error reduction with increasing unknown count. The multigroup energy-discretization method does not exhibit such error reduction (convergence to the analytic solution) until the unknown count is higher than practical—high enough to have more than one unknown per resonance. This has hampered efforts to quantify energy-discretization error except by brute-force comparison against reference solutions of model problems.

Our FEDS method reduces energy discretization error and facilitates its estimation. Figure 35 shows the differences among a straightforward Multigroup (MG) treatment, FEDS-MG (implemented in PDT), and continuous-energy MCNP for two detailed quantities of interest in two slab lattice problems. Important points:

- Integral quantities (multiplication factor, total absorption rate, etc.) are relatively easy for a discretization method to estimate accurately. Detailed quantities, such as the absorption rate in a particular nuclide, particular energy range, and particular spatial sub-volume, are more difficult. Figure 35 considers detailed quantities: absorption rate in $^{238}$U, for neutrons of energy in (154,539) eV, in sub-portions of the fuel in a pin cell.
• Even for such detailed QOIs, FEDS exhibits a monotonically decreasing difference from continuous-energy Monte Carlo as the number of energy unknowns increases. Multigroup (MG) does not (and MG has larger discrepancies).
• Above and below the resolved resonance range, the FEDS and MG calculations shown here used the same group structures and cross sections. The only differences are in the resolved resonance (RR) range.
• Multigroup errors for energies above the RR range cause errors in the downscattering source in the RR range. Thus, even if FEDS were perfect it would still exhibit differences relative to continuous-energy Monte Carlo.
• The MG and FEDS results in Figure 35 employed the same weighting spectra, from NJOY infinite-medium calculations with chord-length-based escape cross sections. Better spectra and better self-shielding methods would improve both MG and FEDS results. The important point, based on both theory and observation, is that FEDS exhibits convergent behavior with O(100) unknowns in the resolved-resonance range, with or without sophisticated spectrum and self-shielding treatments, whereas MG does not exhibit convergent behavior until the number of groups becomes larger than the number of resonances.

![Figure 35. FEDS and MG error as a function of unknown count for two fuel/water lattice problems. Horizontal axis is the inverse of the number of energy unknowns in the resolved resonance (RR) range, which in these problems is from 4.2 eV to 22.7 keV. The QOIs shown are absorption in $^{238}$U in the energy range from 154 eV to 539 eV, for the inner portion of the fuel (left) and the outer portion (right). Results from two slab-geometry lattice problems are shown. Problem A has only $^{238}$U in the fuel. Problem B has both $^{238}$U and $^{235}$U. Other detailed QOIs show similar trends. More integral QOIs (such as $k$ or total absorption in $^{238}$U) show even smoother error-reduction behavior.](Image)

More detail can be found in the references cited previously. FEDS and MG results for detailed and integral QOIs from relevant problems suggest that the results described above are typical: FEDS exhibits convergent error behavior with O(100) RR unknowns while MG does not. This presents the possibility of practical estimates of energy-discretization error for any given problem (even one of a type not encountered previously) without reliance on reference solutions from model problems. For example, the following should yield a reasonable estimate:

1. Let $N_{full}$ = number of energy unknowns in the RR range expected to yield desired accuracy.
2. Solve the problem with FEDS with approximately $N_{full}/2$ energy unknowns.
3. Rerun the problem with FEDS with $N_{\text{full}}$ energy unknowns, using the previous FEDS solution for the initial iterate.
4. Estimate energy discretization error in each QOI by assuming it is first-order (consistent with theory and observation to date) and thus proportional to the inverse of the number of energy unknowns in the RR range.
5. If estimated errors are sufficiently small, exit. If not, or if a more confidence is needed in the error estimate, increase $N_{\text{full}}$ and return to step 3.

The above remarks currently hold only for errors associated with the resolved-resonance range. Treatment of unresolved resonances via FEDS or a similar methodology requires further study.

### VI.4 Spatial and Angular Discretization

It is valuable to have multiple approaches to a complex analysis when bringing up a new capability, which is what we have been doing with PDT during this project. Before we attempted to quantify discretization error, we began our TRIGA calculational effort by comparing results generated by our relatively new PDT capability against those from established codes. During Y1 we made progress on this, with first-year (at that time) grad student Carolyn McGraw responsible for much of the work. We created and implemented DRAGON models for the core, and we developed procedures for transferring DRAGON-generated multigroup cross sections (for both homogenized and heterogeneous pin cells, and for both macroscopic and microscopic cross sections). We developed preliminary PDT models with both heterogeneous and homogeneous pin cells.

During Y2 we devoted significant effort to Monte Carlo neutronics models for the TAMU NSC TRIGA reactor. Our various Monte Carlo models have been useful in directly modeling the state of our core and directly modeling some of our experiments, but in addition they have provided invaluable comparisons as we developed and tested our deterministic alternatives in PDT. We have often employed in PDT the nuclide densities that were determined using the Monte Carlo-based depletion codes.

During Y2 graduate student Jesse Johns made substantial progress on this using both continuous-energy MCNP and continuous-energy Serpent, including coupled nuclide production and depletion with each code. Student Rick Vega also employed KENO for continuous-energy calculations of the neutronics impact of 0.75-inch and 0.5-inch instrumentation tubes. During Y3 Jan Vermaak used both MCNP and Serpent along with the detailed operating history of our (relatively new) LEU core to perform depletion and production calculations, thereby determining the concentrations of important nuclides throughout the core.

During Y2 and Y3 we devoted significant effort to estimating PDT numerical error in steady-state problems as a function of spatial and directional (angular) discretization parameters. Our starting points for this effort were published reactor benchmark problems such as the C5G7 problem. In Y3 we presented a paper at the 2014 Physics of Reactors International Conference, documenting PDT’s accuracy for analysis of water-moderated reactors and serving as an important part of the extensive code- and solution-verification effort that was essential before
PDT could serve its purpose on our project.\textsuperscript{20} In this paper we extensively studied the 2D C5G7 problem\textsuperscript{21} and were happy to find that with PDT we could produce solutions with higher precision than the published MCNP reference solutions. The layout of the C5G7 problem is shown in Figure 36. Examples of the spatial grids we employed for single pincells are shown in Figure 37. The finest grid produces spatial discretization errors of less than 0.005\% in each pin power. In Figure 38 we illustrate the scalar fluxes (for the energy group with the next-to-lowest energies) from our coarsest and finest meshes for the four pincells at the intersection of the four fuel assemblies. Note that the coarse mesh captures the solution quite well.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure36}
\caption{The C5G7 test problem, with overall layout of assemblies and reflector on the left and details of the four assemblies on the right.}
\end{figure}


Figure 37. Spatial grids used for each pincell in the C5G7 problem. The finest mesh had 900 spatial cells per pincell.

Figure 38. Scalar flux from the 6th of the 7 groups (next-to-lowest energy) in the C5G7 problem for the four pins at the intersection of the UOX and MOX assemblies. The finest-mesh solution is on the left and the coarsest-mesh solution is on the right.

Having learned in Y3 the bulk of what we needed to know about spatial and angular discretization error in 2D, in Y4 we turned our attention to the same issue in 3D. We presented a peer-reviewed conference paper at the 2015 ANS Mathematics and Computation conference in
which we demonstrate PDT’s accuracy on the 3D version of the C5G7 problem.\textsuperscript{22} We found that logarithmically spaced axial mesh planes are helpful in resolving the 3D solutions at core/reflector interfaces and at the bottoms of control rods. We have found that the radial mesh requirements and the quadrature-set requirements were approximately the same in 3D as in 2D. An example of one of our discretization-error results is depicted in Figure 39. As we found in 2D, we find that PDT is capable of generating highly accurate reference solutions using its Y2 mesh capability with the linear DFEM spatial discretization method and standard Gauss-Tchebyshhev quadrature sets.

Figure 39. Multiplication factor in 3D C5G7 reactor benchmark problem as a function of number of unknowns per pincell. The horizontal axis is the inverse of that number. Each line shows how $k$ changes as one meshing variable is refined and the others are held fixed, where the variables are: number of polar angles, number of azimuthal angles, number of spatial cells in the radial ($x$-$y$) plane, and number of cells in the axial ($z$) dimension. The black dot is the published reference MCNP solution, with 2-sigma error bars shown.

A summary of our experience with spatial and angular discretization is that if we employ polygonal-prism grids, discontinuous FEMs for spatial differencing, and Gauss-Chebyshev product quadrature sets, our PDT code can generate extremely accurate solutions to 2D and 3D reactor neutronics problems.

VI.5 PDT Computational Performance

We have long demonstrated that our PDT code can achieve excellent parallel efficiency on massively parallel computers for reactor problems with resolved pin-cell geometry. During Y3

we demonstrated excellent scaling out to 256k cores (on the LLNL Vulcan BG/Q machine) on a 3D PWR problem with resolved pins. By excellent scaling we mean a parallel efficiency of 70% relative to an 8-core run. That is, in a weak-scaling reactor problem, sweep time increased by only a factor of \((1.0 / 0.7)\) when we increased core count and problem size by a factor of 32k. This is for full-core boundary-to-boundary sweeps. A key ingredient in this success was the development and implementation of an optimal sweep theory and algorithm, which we described at the 2013 ANS Math and Comp conference.\(^2\) Another key ingredient was the recognition that our provably optimal sweep theory, developed for orthogonal grids, applies to high-fidelity reactor grids if we treat pincells or quarter-pincells, which are orthogonal, as the smallest spatial unit for parallel computation. Because sweeping across a spatial unit (“cell-set”) is executed by a single computational unit (core), or perhaps a set of computational units with access to a shared memory space, the cell-set can contain arbitrary non-orthogonal cells. This is the heart of PDT’s parallel execution of reactor problems.

During Y4 we continued to improve and extend PDT’s single-core and parallel performance. The code’s single-core and 8-core performance was improved in Y4. Further, the code successfully ran neutronics problems with more than 1.5M parallel threads (two threads per core on 768k cores on the Mira BG/Q computer at ANL), with parallel efficiency of >60% relative to an 8-core run. That is the solution time per unknown increased by only a factor of approximately \((1.0 / 0.62)\) when we increase the core count and unknown count by a factor of 96k. Figure 40 shows more results from this scaling study.

We continuously improved PDT’s grind time (time to calculate one unknown during one sweep) over the course of the project, in addition to pushing its excellent parallel scaling out to higher process counts. Figure 41 shows how PDT’s time per unknown has dropped over time on the BlueGene/Q platform, and shows that the code now scales quite well out to approximately 1M cores. Time per unknown on 768k cores is now approximately three times faster than was serial time per unknown at the start of the project.

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Figure 40. Parallel efficiency as a function of number of parallel threads for a “weak-scaling” suite with a fixed number of unknowns per thread. Test problem had only a single energy group and 80 total quadrature directions, with 4096 cells per thread. Computations were run on the Mira BG/Q machine at ANL.

Figure 41. History of PDT “grind times”: time to execute a full-domain boundary-to-boundary sweep, per unknown, per core. Desired curve is low and flat. Most recent results are green squares. PDT performance improved significantly (lower, flatter curve) during the course of the project.

VII  Heat Transfer and Fluid Flow

We planned from the project’s start that our highest-fidelity heat-transfer and fluid-flow capability would be provided by the STAR-CCM+ code, a commercial product of CD-
ADAPCO. We also determined early on that a simpler heat-transfer and fluid-flow capability would be of great utility. During Y2 we used COBRA-TF, a subchannel code that is also used by the CASL hub, for most of the thermal-hydraulics calculations in that year’s safety analysis of our incore guide tubes.

Figure 42 shows the layout of our TRIGA core, with fuel bundles located in columns 2-7 and rows B-F. In one COBRA-TF calculated scenario, bundles E5, E6, F5, and F6 were modeled, with the heating rate for each pin taken from a full-core MCNP neutronics calculation and the axial profile taken to be constant. One calculation simulated no blockage, which represents the unmodified (no-guide-tube) state. Another calculation simulated blockage by five proposed instrument tubes, which are shown in black in Figure 43. As Figure 43 illustrates, the blockage resulted in a 7.6°C increase in the hottest channel of these four bundles (channel 21) and a 0.3°C increase at the centerline of the hottest rod (rod 13 – the only rod touching channel 21). The largest temperature increase for any channel was 9.4°C and the largest percentage increase was 12.8%.
The calculations were repeated with realistic axial power profiles for each pin, again taken from a detailed MCNP calculation. Again, one calculation simulated no blockage and the other simulated blockage by five proposed instrument tubes (with blocked channels shown in black in Figure 44). The blockage resulted in a 7.9°C increase in the hottest channel of these four bundles (channel 21) and a 0.3°C increase at the centerline of the hottest rod (rod 13 – the only rod touching channel 21). The largest temperature increase for any channel was 8.1°C and the largest percentage increase was 10.9%.

Figure 44. Results with no blockage (left) and with five corner locations blocked (right), assuming realistic axial power profiles.

During Y3 we made progress using both COBRA-TF and STAR-CCM+ to analyze steady-state natural-circulation thermal-hydraulics in our TRIGA reactor, both with and without guide tubes displacing coolant. Results are reported in a peer-reviewed conference paper that was presented at the PHYSOR 2014 conference.1

During Y4 we began using both STAR-CCM+ and RELAP5 to model the heat transfer and fluid flow in the TRIGA, with and without instrumentation tubes. Some the results are reported in a publication cited previously.2

VIII Coupled Simulations

We determined during the course of the project that a fruitful path forward was to add heat-conduction capability to the PDT particle-transport code. This should allow reasonably accurate calculation of rapid transients such as high-reactivity pulses, in which there is not enough time for thermal energy to conduct or convect very far.

Pulsing operations begin with the reactor at steady state at a low power, usually a few hundred watts. The “transient” control rod is ejected using compressed CO₂, quickly placing the reactor into a prompt-supercritical state. Neutron population, power, and fuel temperature rise substantially over the course of several milliseconds. Increased temperature in the fuel leads to negative reactivity insertion, and the neutron population and power quickly drop.
Our “pulse-mode” PDT calculation aims to model this as follows:

- A $k$-eigenvalue calculation is performed at the initial low-power condition and the eigenfunction is normalized to be consistent with the correct power level.
- A time-dependent calculation is initiated as follows:
  - The angular flux is initialized to the normalized $k$-eigenfunction.
  - Temperatures in all materials are initialized to pool temperature (because initial power is too low to make them higher).
  - A fixed neutron source-rate density in each spatial cell in the fuel is set to the delayed-neutron source-rate density that is consistent with the normalized eigenfunction, divided by the initial calculation’s calculated $k$. (The reason for the division by $k$ is discussed below.)
  - The fission term is set to model only prompt neutron emission, with the prompt “nu” value divided by the initial calculation’s calculated $k$ and the spectrum consistent with only prompt neutrons.
- Several time steps of coupled neutronics/heat-conduction are run to verify that temperatures and fluxes remain constant. This should be the case if the original $k$-eigenvalue problem was converged properly, even if $k$ is not calculated to be exactly unity, because the divisions by $k$ described above create a fixed-source problem steady-state problem that is satisfied by the eigenfunction.
- The transient rod ejection begins, and the time-dependent simulation continues.

In this model, the transient is assumed to be sufficiently rapid that the delayed-neutron source remains constant for the (several-millisecond) time period of interest. Energy from fission is deposited rapidly by fission fragments, gammas, and neutrons, and the conduction equation calculates temperature increases under the assumption that convective heat transfer coefficients at pin/coolant interface remain fixed during the same short time period.

Early in Y5 we tested a continuous finite-element conduction solver with a novel “twist” that models the temperature drop across the “gap” between the fuel meat and the cladding as a discontinuity. Results were quite accurate, as shown in Figure 45.
Later in the year we implemented the heat-conduction model into PDT, first as a standalone heat-conduction solver for the fuel/cladding system and later for coupled neutronics/conduction problems. Results from single-pin-cell verification tests are shown for problems with and without a gap between the fuel and cladding in Figure 46 and Figure 47, respectively. Results agree with theory within numerical error, which was quite small for the mesh that was used (and shown in the figures) here.
By the time the project ran out of time, we were still debugging the coupled neutronics/conduction methodology, and thus unfortunately do not have results to show. We do expect to complete this and report on it in a peer-reviewed conference paper at an ANS conference in the near future.